Condensed Matter Physics II. – A.A. 2010-2011, February 24, 2012

(time 3 hours)

Solve the following two exercises, each has a maximum score of 18 for a total of 36. A score between 33 e 36 corresponds to 30 cum laude, between 30 e 32 is renormalized to 30 (the maximum official score, without laude).

NOTE:

- Give all details which help in understanding the proposed solution. Answers which only contain the final result or not enough detail will be judged insufficient and discarded;
- If you are requested to give evaluation/estimates, do so using 3 significant figures.

Exercise 1: *Nearest-neighbors phonons*

Consider the atoms on a Bravais lattice and small deviations $\mathbf{u}(\mathbf{R})$ from the equilibrium positions $\mathbf{R}$. In the nearest-neighbors approximation the potential energy is approximated by

$$U = \frac{K}{4\mathrm{d}^2}\sum_{\mathbf{R}}\sum_{\mathbf{d}}[(\mathbf{u}_{\mathbf{R}+\mathbf{d}} - \mathbf{u}_{\mathbf{R}})\cdot\mathbf{d}]^2,$$

where the second sum (over $\mathbf{d}$) runs over the nearest neighbors of the lattice site $\mathbf{R}$.

1. Calculate
$$\frac{\partial U}{\partial u_{\alpha,\mathbf{R}'}},$$
where $u_{\alpha,\mathbf{R}'}$ is the cartesian α-component of $\mathbf{u}_{\mathbf{R}'}$.
2. Using the previous result calculate
$$D_{\alpha,\beta}(\mathbf{R}' - \mathbf{R}'') = \frac{\partial^2 U}{\partial u_{\beta,\mathbf{R}''}\partial u_{\alpha,\mathbf{R}'}}.$$
3. Specialize to a two-dimensional square lattice with lattice spacing a and calculate explicitly the four elements of $D_{\alpha,\beta}(\mathbf{R}' - \mathbf{R}'')$.
4. Calculate now the so-called dynamical matrix
$$D_{\alpha,\beta}(\mathbf{q}) = \sum_{\mathbf{R}''} D_{\alpha,\beta}(\mathbf{R}' - \mathbf{R}'')e^{-i\mathbf{q}\cdot(\mathbf{R}'-\mathbf{R}'')}.$$
5. Obtain the eigenvalues and eigenvectors (polarization vectors) of the above matrix.
6. Calculate the phonon density of states,
$$g(\omega) = \sum_{i=1,2}\left[\frac{1}{A}\sum_{\mathbf{q}\in FBZ}\delta(\omega - \omega_i(\mathbf{q}))\right],$$
as function of ω specifying the admissable values for ω; here $\omega_i(\mathbf{q})$, i=1,2, are the two phonon branches found from the eigenvalues of the dynamical matrix.

Esercizio 2 *Pauli susceptibility in 3D at $T \neq 0$*

Consider a non interacting electron gas in 3 dimensions, in a uniform magnetic field $\mathbf{H} = H\hat{z}$. The energy levels of the $\sigma = \pm$ (i.e., up or down) spin electrons are $e_\sigma(\mathbf{k}, H) = \hbar^2 k^2/(2m) + \sigma\mu_B H$. We shall denote with n the number density and V the volume of the sample.

1. Knowing that total density of states at $H = 0$,
$$g_0(E) = \frac{2}{V}\sum_{\mathbf{k}} \delta(E - \frac{\hbar^2 k^2}{2m}) = \frac{3}{2}\frac{n}{E_F}\sqrt{\frac{E}{E_F}}\theta(E),$$
express
$$g_\sigma(E, H) = \frac{1}{V}\sum_{\mathbf{k}} \delta(E - e_\sigma(\mathbf{k}))$$
in terms of $g_0(E)$. Here, $\theta(x)$ is the Heaviside step function.
2. Demonstrate that the density of σ electrons at givel T, H, μ
$$n_\sigma(T, H, \mu) = \int dE \, \frac{g_\sigma(E, H)}{exp[\beta(E - \mu)] + 1},$$
can be expressed in terms of that at $H = 0$ at a shifted chemical potential $\tilde{\mu} = \mu - \sigma\mu_B H$, i.e.,
$$n_\sigma(T, H, \mu) = n_\sigma(T, 0, \tilde{\mu}) = \int_0^\infty dE \, \frac{g_0(E)/2}{exp[\beta(E - \tilde{\mu})] + 1}.$$
This is easily shown by considering a change ov variable in the integral.
3. Assume $T \ll T_F$ and use Sommerfeld expansion (see below) to calculate $n_\sigma(T, H, \mu)$.
4. Use the result above to calculate $M(T, H, \mu) = -\mu_B(n_+ - n_-)$.
5. Assuming that $\mu(T, H) = \mu_0(T) + \alpha H^2, \quad H \to 0$, expand M to linear order in H.
6. Evaluate the spin susceptibilty
$$\chi_S = \left.\frac{\partial M}{\partial H}\right|_{H=0}$$
and rewrite it to display the fractional change of χ_S due to the small but finite temperature.

Note: Sommerfeld expansion, valid for $f(E)$ a smooth function, slow with respect to the exponential and $\exp \beta\mu \gg 1$, is
$$\int_0^\infty dE \frac{f(E)}{exp[\beta(E - \mu)] + 1} = \int_0^\mu dE f(E) + \frac{\pi^2}{6}(K_B T)^2 f'(\mu) + \dots \; .$$